

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: S. Kumar Examiner #: 69594 Date: 2/24/04
 Art Unit: 162 Phone Number: 302-6040 Serial Number: 09/826287
 Mail Box and Bldg/Room Location: REM 5DE1 Results Format Preferred (circle): PAPER DISK E-MAIL
5C18

If more than one search is submitted, please prioritize searches in order of need.

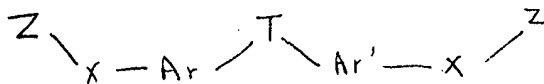
 Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Generation of Combinatorial Synthetic Libraries

Inventors (please provide full names): Randall S. Alberte et al.

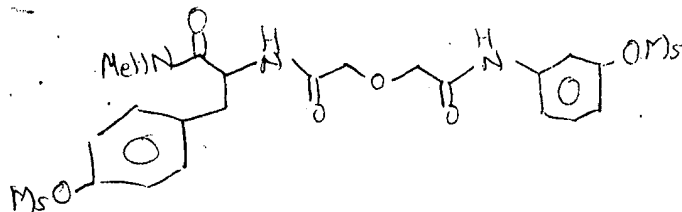
Earliest Priority Filing Date: 4/3/2000

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



X is O, S, NR' or bond
 Z R, acyl, trialkylsilyl, alkylsulfonyle, fluoroalkylsulfonyle, SCO₂OH, amylsulfonyle
 Ar, Ar' are optionally subst. aryl or heteroaryl
 T is covalent tether connecting Ar & Ar', the linker is selected from amide, ether, amine or ester
 R H, alkyl, alkenyl, aryl, aralkyl, formyl, acyl, sulfonyle etc.

Species



See claims 1-19

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>am</u>	NA Sequence (#) _____	STN <u>✓</u>
Searcher Phone #: <u>27504</u>	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>✓</u>	Questel/Orbit _____
Date Searcher Picked Up: <u>2/28</u>	Bibliographic _____	Dr. Link _____
Date Completed: <u>2/28</u> (SIS)	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: _____	Fulltext _____	Sequence Systems _____
Clerical Prep Time: <u>15</u> FEB 24 2004	Patent Family _____	WWW/Internet _____
Online Time: <u>1:30</u>	Other _____	Other (specify) _____

=> d his

(FILE 'HOME' ENTERED AT 10:27:54 ON 28 FEB 2004)
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 10:28:03 ON 28 FEB 2004

L1 1 S US20020052003/PN OR WO2001-US10969/AP,PRN
E ALBERTE R/AU
L2 100 S E4-E6
E SMITH R/AU
L3 931 S E3,E37-E43
E SMITH ROBERT/AU
L4 103 S E3
E SMITH ROBERT D/AU
L5 44 S E3-E7
E SMITH ROB/AU
L6 5 S E3
E SMITH BOB/AU
L7 7 S E3,E8
E PHYCOGEN/PA,CS
L8 7 S E3-E8
L9 7 S L1-L7 AND L8
L10 1 S L1 AND L9
SEL RN

FILE 'REGISTRY' ENTERED AT 10:30:21 ON 28 FEB 2004

L11 4 S E1-E4

FILE 'HCAPLUS' ENTERED AT 10:31:51 ON 28 FEB 2004

L12 6 S L9 NOT L10
SEL RN

FILE 'REGISTRY' ENTERED AT 10:32:00 ON 28 FEB 2004

L13 69 S E5-E73
L14 67 S L13 NOT L11
L15 10 S L14 AND NR>=2
L16 2 S L13 NOT L14
L17 2 S L11 NOT L16
L18 4 S L11,L16,L17

FILE 'HCAPLUS' ENTERED AT 10:34:14 ON 28 FEB 2004

L19 8 S L2 AND L3-L7
L20 5 S L19 NOT L9
SEL RN

FILE 'REGISTRY' ENTERED AT 10:34:49 ON 28 FEB 2004

L21 18 S E74-E91
L22 1 S L21 AND NR>=2

FILE 'HCAOLD' ENTERED AT 10:35:08 ON 28 FEB 2004

L23 0 S L18

FILE 'HCAPLUS' ENTERED AT 10:35:10 ON 28 FEB 2004

L24 2 S L18
L25 2 S L24 AND L1-L10

FILE 'USPATFULL, USPAT2' ENTERED AT 10:35:29 ON 28 FEB 2004

L26 1 S L18

FILE 'HCAPLUS' ENTERED AT 10:39:00 ON 28 FEB 2004

L27 1170 S L2-L8 NOT L10,L12,L20
L28 6 S L27 AND (BENZENE? OR HETERO?)/SC,SX
L29 4 S L28 NOT (75 OR 29)/SC

L30 7 S L27 AND (25 OR 27)/SC,SX
L31 1 S L30 NOT L28
SEL RN L29

FILE 'REGISTRY' ENTERED AT 10:42:08 ON 28 FEB 2004

L32 91 S E93-E183
L33 66 S L32 AND NR>=2

FILE 'HCAPLUS' ENTERED AT 10:43:21 ON 28 FEB 2004

L34 1163 S L27 NOT L28-L31
L35 2 S L34 AND LIBRARY
L36 2 S L34 AND COMBINATOR?
L37 3 S L34 AND SOLID PHASE
L38 7 S L35-L37
L39 1 S L34 AND 21/SC,SX
L40 1 S L34 AND HIGH THROUGHPUT
L41 0 S L34 AND HIGH THROUGH PUT
L42 0 S L34 AND HTS
L43 13 S L34 AND SCREEN?
L44 1 S L40 AND L43
L45 0 S L34 AND SCAFFOLD?
L46 12 S L34 AND ?ARRAY?

=> fil reg

FILE 'REGISTRY' ENTERED AT 10:47:54 ON 28 FEB 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 27 FEB 2004 HIGHEST RN 655785-05-0

DICTIONARY FILE UPDATES: 27 FEB 2004 HIGHEST RN 655785-05-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide can tot l18

L18 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2004 ACS on STN

RN 365240-90-0 REGISTRY

CN Carbamic acid, [(1S)-2-(methylamino)-2-oxo-1-[[4-(sulfooxy)phenyl]methyl]ethyl]-, C-(phenylmethyl) ester, monoammonium salt
(9CI) (CA INDEX NAME)

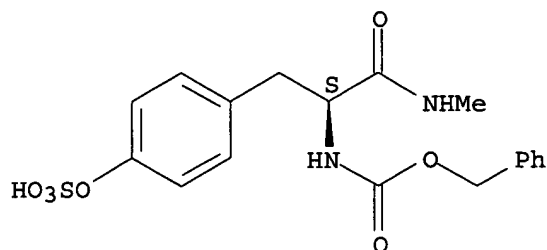
FS STEREOSEARCH

MF C18 H20 N2 O7 S . H3 N

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



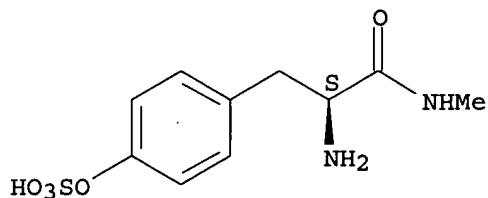
● NH₃

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:288577

L18 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2004 ACS on STN
RN 365240-89-7 REGISTRY
CN Benzenepropanamide, α -amino-N-methyl-4-(sulfooxy)-, monoammonium salt, (α S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C10 H14 N2 O5 S . H3 N
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
CRN (108050-90-4)

Absolute stereochemistry.



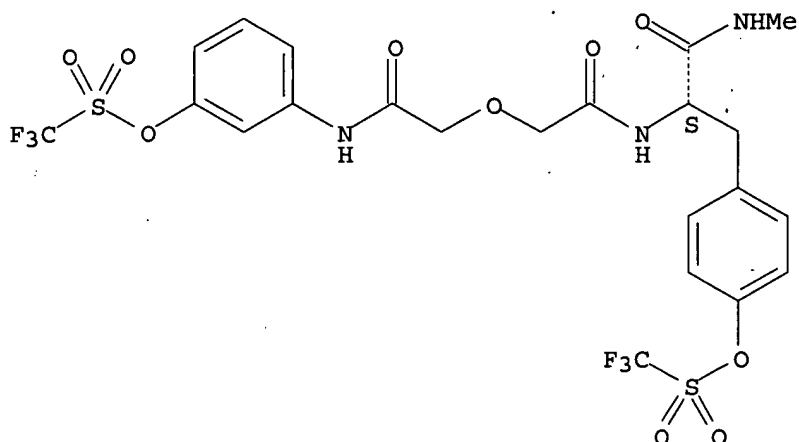
● NH₃

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:288577

L18 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2004 ACS on STN
RN 365240-88-6 REGISTRY
CN Methanesulfonic acid, trifluoro-, 4-[(2S)-3-(methylamino)-3-oxo-2-[[[2-oxo-2-[[3-[[[(trifluoromethyl)sulfonyl]oxy]phenyl]amino]ethoxy]acetyl]amino]propyl]phenyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H21 F6 N3 O10 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:252981

REFERENCE 2: 135:288577

L18 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2004 ACS on STN

RN 365240-87-5 REGISTRY

CN Benzenepropanamide, N-methyl-4-[(methanesulfonyl)oxy]-α-[[[2-[[3-[(methanesulfonyl)oxy]phenyl]amino]-2-oxoethoxy]acetyl]amino]-, (αS)- (9CI) (CA INDEX NAME)

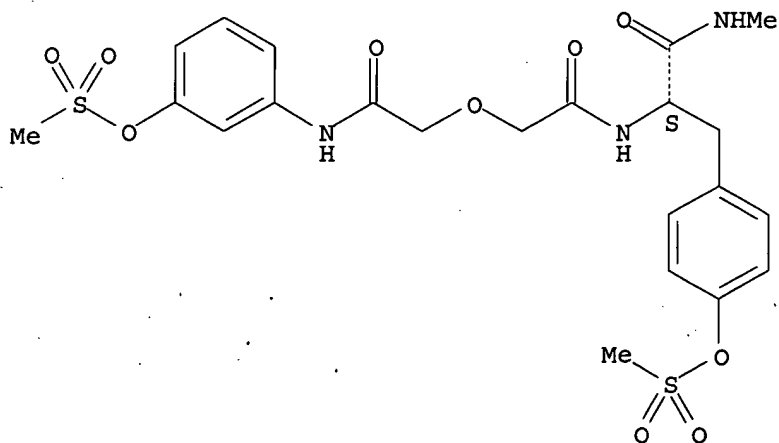
FS STEREOSEARCH

MF C22 H27 N3 O10 S2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:252981

REFERENCE 2: 135:288577

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 10:48:06 ON 28 FEB 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 28 Feb 2004 VOL 140 ISS 10

FILE LAST UPDATED: 27 Feb 2004 (20040227/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all hitstr tot 125

L25 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:716026 HCAPLUS

DN 137:252981

ED Entered STN: 20 Sep 2002

TI Monomer or polymer-based anti-adhesive compounds

IN **Alberte, Randall S.; Smith, Robert D.**PA **Phycogen, Inc., USA; Cerno Biosciences LLC**

SO PCT Int. Appl., 62 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 1, 10, 19

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002072020	A2	20020919	WO 2002-US7426	20020312
	WO 2002072020	A3	20031127		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP	1385821	A2	20040204	EP 2002-725119	20020312

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRAI US 2001-275223P P 20010312

WO 2002-US7426 W 20020312

OS MARPAT 137:252981

AB Compds. which exhibit anti-adhesive properties are described. The compds. may be monomers or polymers. Methods for treating receptor mediated diseases are provided by using compds. of the invention. Further methods are provided for crop protection, medical devices and anti-fouling. Sulfated L-tyrosine showed anti-adhesive activity in the Staphylococcus assay.

ST antiadhesive monomer polymer; antifouling monomer polymer

IT Adhesion, biological

Antifouling agents

Colletotrichum acutatum

Medical goods

Pseudoalteromonas atlantica

Staphylococcus epidermidis

(monomer or polymer-based anti-adhesive compds.)

IT Polymers, biological studies

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(monomer or polymer-based anti-adhesive compds.)

IT 956-46-7 9003-53-6, Polystyrene 9080-79-9, Poly(styrenesulfonic acid)

sodium salt 26795-32-4D, sulfonated, sodium salt 28038-50-8,

Poly(4-styrenesulfonic acid) sodium salt 63589-56-0 73260-43-2

104983-61-1, Maleic acid-styrenesulfonic acid copolymer sodium salt

142847-49-2, L-Tyrosine hexamer 365240-87-5 365240-88-6

460061-89-6 460061-90-9

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(monomer or polymer-based anti-adhesive compds.)

IT 365240-87-5 365240-88-6

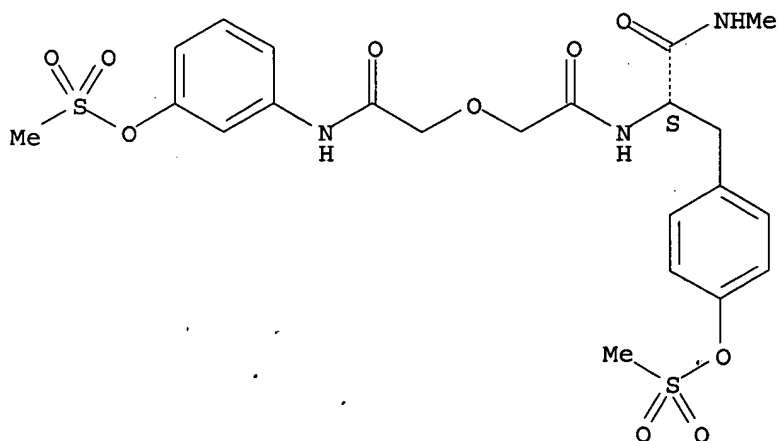
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(monomer or polymer-based anti-adhesive compds.)

RN 365240-87-5 HCAPLUS

CN Benzenepropanamide, N-methyl-4-[(methylsulfonyl)oxy]- α -[[[2-[[3-[(methylsulfonyl)oxy]phenyl]amino]-2-oxoethoxy]acetyl]amino]-, (α S)-(9CI) (CA INDEX NAME)

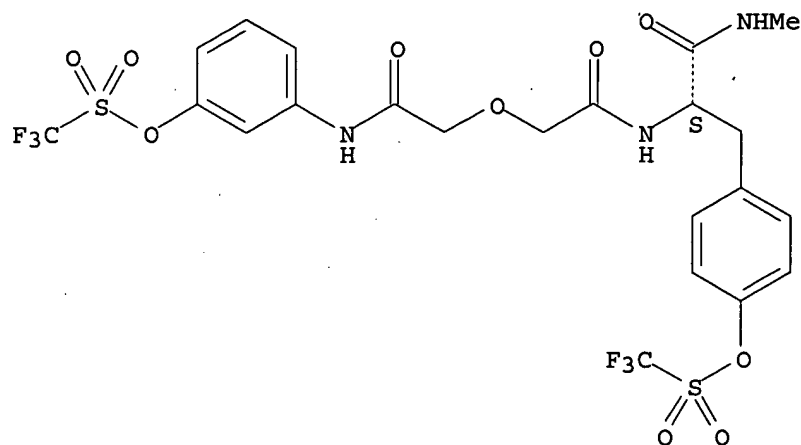
Absolute stereochemistry.



RN 365240-88-6 HCAPLUS

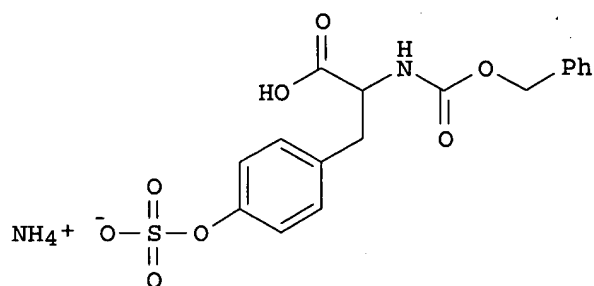
CN Methanesulfonic acid, trifluoro-, 4-[(2S)-3-(methylamino)-3-oxo-2-[[[2-oxo-2-[[3-[[[(trifluoromethyl)sulfonyl]oxy]phenyl]amino]ethoxy]acetyl]amino]propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L25 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN.
 AN 2001:747740 HCAPLUS
 DN 135:288577
 ED Entered STN: 12 Oct 2001
 TI Generation of combinatorial synthetic libraries (e.g. sulfonyloxy-arylalkyloxy-sulfones) and screening for proadhesins and nonadhesins
 IN Alberte, Randall S.; Smith, Robert D.
 PA Phycogen, Inc., USA
 SO PCT Int. Appl., 88 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07C305-24
 ICS C07D211-22; C07D207-08; C07D395-08; C07D303-46; A01N041-02;
 A01N043-36; A01N043-40; A01N043-60; A01N043-02
 CC 25-13 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 10, 21
 FAN.CNT 1

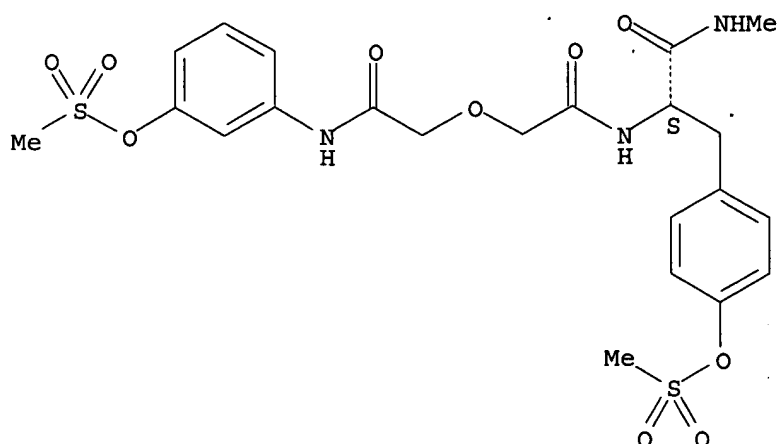
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001074762	A2	20011011	WO 2001-US10969	20010403 <--
WO 2001074762	A3	20020530		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002052003	A1	20020502	US 2001-826287	20010403 <--
PRAI US 2000-194333P	P	20000403		
OS MARPAT 135:288577				
GI				



II

- AB (Libraries of) title compds. Z-X-Ar-T-Ar1-X-Z [X = bond, O, S, or NR1; Z = H, acyl, trialkylsilyl, alkylsulfonyl, fluoroalkylsulfonyl, arylsulfonyl, S(O)OH; Ar and Ar1 = (un)substituted (hetero)aryl; T = covalent tether connecting Ar and Ar', wherein said covalent linker comprises an amide, ether, amine or ester moiety; R = H, alkyl, aryl, aralkyl; R1 = H, alk(en)yl, aryl, aralkyl, formyl, acyl, sulfonyl, (CH)mR2; R2 = aryl, cycloalkyl, cycloalkenyl, heterocyclyl; m = 0 - 8; I] were prepared and used to enhance or inhibit bioadhesion to a surface. Four synthetic examples were disclosed and screened for cellular adhesion to polystyrene. E.g. II, 0.5%aq in a polypropylene microplate resulted in inhibition of adhesion of *Staphylococcus epidermidis* (74%) and *Pseudoalteromonas atlantica* (32%). Claimed uses of compds. of the invention include inhibition of adhesion to a surface by a bacterium, fungus, virion, etc., where the surface is: an aquatic vessel, an off-shore platform, a portion of a human cell membrane, etc.
- ST sulfone sulfonate amide bioadhesion prepn
- IT Adhesion, biological
Cell adhesion
Combinatorial library
Solid phase synthesis
(generation of combinatorial synthetic libraries (e.g. sulfonyloxy-arylalkyloxy-sulfones) and screening for proadhesins and nonadhesins)
- IT Adhesins
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(proadhesins; generation of combinatorial synthetic libraries (e.g. sulfonyloxy-arylalkyloxy-sulfones) and screening for proadhesins and nonadhesins)
- IT 365240-87-5 365240-88-6 365240-89-7
365240-90-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(generation of combinatorial synthetic libraries (e.g. sulfonyloxy-arylalkyloxy-sulfones) and screening for proadhesins and nonadhesins)
- IT 365240-87-5 365240-88-6 365240-89-7
365240-90-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(generation of combinatorial synthetic libraries (e.g. sulfonyloxy-arylalkyloxy-sulfones) and screening for proadhesins and nonadhesins)
- RN 365240-87-5 HCAPLUS
- CN Benzenepropanamide, N-methyl-4-[(methylsulfonyl)oxy]-α-[[[2-[[3-[(methylsulfonyl)oxy]phenyl]amino]-2-oxoethoxy]acetyl]amino]-, (αS)-(9CI) (CA INDEX NAME)

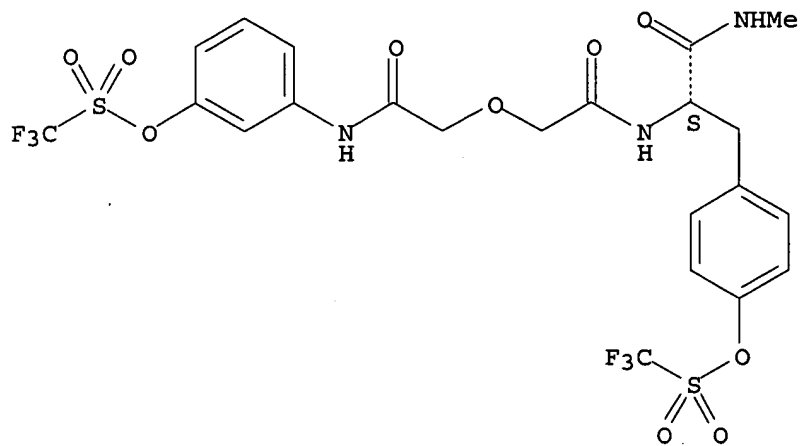
Absolute stereochemistry.



RN 365240-88-6 HCAPLUS

CN Methanesulfonic acid, trifluoro-, 4-[(2S)-3-(methylamino)-3-oxo-2-[[[2-oxo-2-[[3-[[[(trifluoromethyl)sulfonyl]oxy]phenyl]amino]ethoxy]acetyl]amino]propyl]phenyl ester (9CI) (CA INDEX NAME)

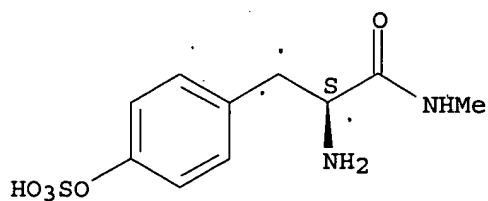
Absolute stereochemistry.



RN 365240-89-7 HCAPLUS

CN Benzenepropanamide, α -amino-N-methyl-4-(sulfooxy)-, monoammonium salt, (α S)- (9CI) (CA INDEX NAME)

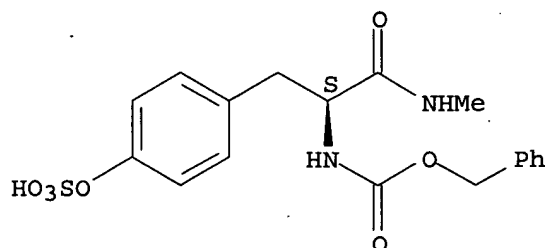
Absolute stereochemistry.



● NH₃

RN 365240-90-0 HCAPLUS
 CN Carbamic acid, [(1S)-2-(methylamino)-2-oxo-1-[[4-(sulfooxy)phenyl]methyl]ethyl]-, C-(phenylmethyl) ester, monoammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> fil uspatall

FILE 'USPATFULL' ENTERED AT 10:48:36 ON 28 FEB 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 10:48:36 ON 28 FEB 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs hitstr l26

L26 ANSWER 1 OF 1 USPATFULL on STN

AN 2002:99107 USPATFULL

TI Generation of combinatorial synthetic libraries and screening for proadhesins and nonadhesins

IN Alberte, Randall S., Falmouth, ME, UNITED STATES

Smith, Robert D., Falmouth, ME, UNITED STATES

PI US 2002052003 A1 20020502

AI US 2001-826287 A1 20010403 (9)

PRAI US 2000-194333P 20000403 (60)

DT Utility

FS APPLICATION

LREP FOLEY, HOAG & ELIOT, LLP, PATENT GROUP, ONE POST OFFICE SQUARE, BOSTON, MA, 02109

CLMN Number of Claims: 40

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 2739

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB One aspect of the present invention relates to compounds, comprising at least two moieties selected from the group consisting of aryl sulfonates and aryl sulfates. A second aspect of the present invention relates to combinatorial libraries of the aforementioned compounds. The present invention also relates to compositions comprising a compound of the present invention. A fourth aspect of the present invention relates to the use of a compound or composition of the present invention in a method for inhibiting bioadhesion to a surface. Another aspect of the present invention relates to the use of a compound or composition of the present invention in a method for enhancing bioadhesion to a surface.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 365240-87-5 365240-88-6 365240-89-7

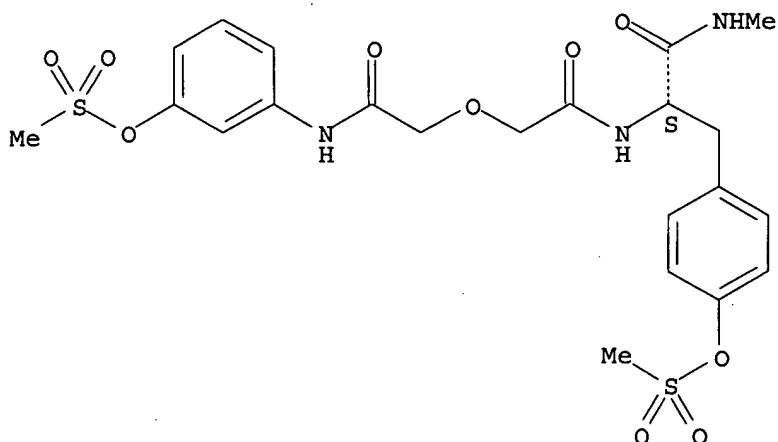
365240-90-0

(generation of combinatorial synthetic libraries (e.g. sulfonyloxy-arylalkyloxy-sulfones) and screening for proadhesins and nonadhesins)

RN 365240-87-5 USPTAFULL

CN Benzenepropanamide, N-methyl-4-[(methylsulfonyl)oxy]- α -[[[2-[[3-[(methylsulfonyl)oxy]phenyl]amino]-2-oxoethoxy]acetyl]amino]-, (α S) - (9CI) (CA INDEX NAME)

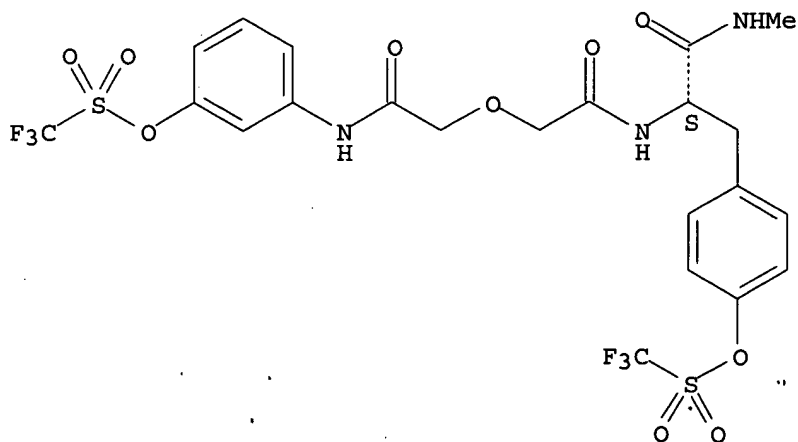
Absolute stereochemistry.



RN 365240-88-6 USPTAFULL

CN Methanesulfonic acid, trifluoro-, 4-[(2S)-3-(methylamino)-3-oxo-2-[[[2-oxo-2-[[3-[[[(trifluoromethyl)sulfonyl]oxy]phenyl]amino]ethoxy]acetyl]amino]propyl]phenyl ester (9CI) (CA INDEX NAME)

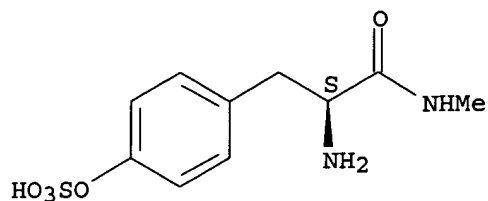
Absolute stereochemistry.



RN 365240-89-7 USPTAFULL

CN Benzenepropanamide, α -amino-N-methyl-4-(sulfooxy)-, monoammonium salt, (α S) - (9CI) (CA INDEX NAME)

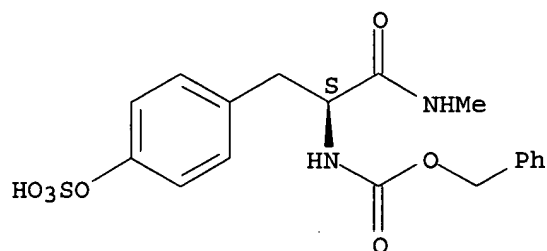
Absolute stereochemistry.



● NH₃

RN 365240-90-0 USPATFULL
 CN Carbamic acid, [(1S)-2-(methylamino)-2-oxo-1-[[4-(sulfooxy)phenyl]methyl]ethyl]-, C-(phenylmethyl) ester, monoammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● NH₃

=> fil hcplus
 FILE 'HCAPLUS' ENTERED AT 10:48:56 ON 28 FEB 2004
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 28 Feb 2004 VOL 140 ISS 10
 FILE LAST UPDATED: 27 Feb 2004 (20040227/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all l44

L44 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:1004134 HCAPLUS
ED Entered STN: 26 Dec 1995
TI **High throughput** whole cell **screens** for drug
discovery: feasibility and utility
AU McKernan, Patricia; **Smith, Robert**; Rosenberg, Gareth; Piggott,
James
CS ZymoGenetics, Inc., Seattle, WA, USA
SO Medicinal Chemistry Research (1995), 5(8), 646
CODEN: MCREEB; ISSN: 1054-2523
PB Birkhaeuser
DT Journal; Miscellaneous
LA English
AB Unavailable

=> => fil reg

FILE 'REGISTRY' ENTERED AT 10:54:01 ON 28 FEB 2004
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 27 FEB 2004 HIGHEST RN 655785-05-0
DICTIONARY FILE UPDATES: 27 FEB 2004 HIGHEST RN 655785-05-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide can tot

L61 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN
RN **946-80-5** REGISTRY
CN Benzene, (phenoxymethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ether, benzyl phenyl (6CI, 7CI, 8CI)
OTHER NAMES:
CN Anisole, α -phenyl-
CN Benzyl phenyl ether
CN Benzyloxybenzene
CN NSC 77971
CN Phenyl benzyl ether
FS 3D CONCORD
MF C13 H12 O
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
CHEMINFORMRX, CSChem, DETHERM*, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB,
SPECINFO, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

PhO-CH₂-Ph

****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

503 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
503 REFERENCES IN FILE CAPLUS (1907 TO DATE)
42 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 140:128110
REFERENCE 2: 140:95523
REFERENCE 3: 140:76686
REFERENCE 4: 140:6141
REFERENCE 5: 139:327472
REFERENCE 6: 139:324980
REFERENCE 7: 139:307582
REFERENCE 8: 139:247161
REFERENCE 9: 139:181971
REFERENCE 10: 139:113495

L61 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN

RN 122-39-4 REGISTRY

CN Benzenamine, N-phenyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Diphenylamine (8CI)

OTHER NAMES:

CN Anilinobenzene

CN Benzene, (phenylamino)-

CN DBA

CN DFA

CN DPA

CN N,N-Diphenylamine

CN N-Phenylaniline

CN N-Phenylbenzenamine

CN Naugalube 428L

CN No-Scald

CN NSC 215210

FS 3D CONCORD

MF C12 H11 N

CI COM

LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VETU, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

Ph-NH-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8113 REFERENCES IN FILE CA (1907 TO DATE)
547 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
8123 REFERENCES IN FILE CAPLUS (1907 TO DATE)
14 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 140:148598
REFERENCE 2: 140:147425
REFERENCE 3: 140:146995
REFERENCE 4: 140:146994
REFERENCE 5: 140:146674
REFERENCE 6: 140:130881
REFERENCE 7: 140:130864
REFERENCE 8: 140:129555
REFERENCE 9: 140:129058
REFERENCE 10: 140:128164

L61 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN

RN 93-99-2 REGISTRY

CN Benzoic acid, phenyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Phenol, benzoate (7CI)

OTHER NAMES:

CN NSC 37086

CN Phenyl benzoate

FS 3D CONCORD

MF C13 H10 O2

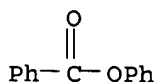
CI COM

LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DETHERM*, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, PROMT, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1068 REFERENCES IN FILE CA (1907 TO DATE)

50 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1071 REFERENCES IN FILE CAPLUS (1907 TO DATE)
45 REFERENCES IN FILE CAGLD (PRIOR TO 1967)

REFERENCE 1: 140:130808
REFERENCE 2: 140:129134
REFERENCE 3: 140:127836
REFERENCE 4: 140:111435
REFERENCE 5: 140:111130
REFERENCE 6: 140:95523
REFERENCE 7: 140:93750
REFERENCE 8: 140:93729
REFERENCE 9: 140:61428
REFERENCE 10: 140:43540

=> => d his

(FILE 'HOME' ENTERED AT 10:27:54 ON 28 FEB 2004)
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 10:28:03 ON 28 FEB 2004

L1 1 S US20020052003/PN OR WO2001-US10969/AP,PRN
E ALBERTE R/AU
L2 100 S E4-E6
E SMITH R/AU
L3 931 S E3,E37-E43
E SMITH ROBERT/AU
L4 103 S E3
E SMITH ROBERT D/AU
L5 44 S E3-E7
E SMITH ROB/AU
L6 5 S E3
E SMITH BOB/AU
L7 7 S E3,E8
E PHYCOGEN/PA,CS
L8 7 S E3-E8
L9 7 S L1-L7 AND L8
L10 1 S L1 AND L9
SEL RN

FILE 'REGISTRY' ENTERED AT 10:30:21 ON 28 FEB 2004

L11 4 S E1-E4

FILE 'HCAPLUS' ENTERED AT 10:31:51 ON 28 FEB 2004

L12 6 S L9*NOT L10
SEL RN

FILE 'REGISTRY' ENTERED AT 10:32:00 ON 28 FEB 2004

L13 69 S E5-E73
L14 67 S L13 NOT L11
L15 10 S L14 AND NR>=2
L16 2 S L13 NOT L14
L17 2 S L11 NOT L16

L18 4 S L11,L16,L17

FILE 'HCAPLUS' ENTERED AT 10:34:14 ON 28 FEB 2004

L19 8 S L2 AND L3-L7

L20 5 S L19 NOT L9
SEL RN

FILE 'REGISTRY' ENTERED AT 10:34:49 ON 28 FEB 2004

L21 18 S E74-E91

L22 1 S L21 AND NR>=2

FILE 'HCAOLD' ENTERED AT 10:35:08 ON 28 FEB 2004

L23 0 S L18

FILE 'HCAPLUS' ENTERED AT 10:35:10 ON 28 FEB 2004

L24 2 S L18

L25 2 S L24 AND L1-L10

FILE 'USPATFULL, USPAT2' ENTERED AT 10:35:29 ON 28 FEB 2004

L26 1 S L18

FILE 'HCAPLUS' ENTERED AT 10:39:00 ON 28 FEB 2004

L27 1170 S L2-L8 NOT L10,L12,L20

L28 6 S L27 AND (BENZENE? OR HETERO?)/SC,SX

L29 4 S L28 NOT (75 OR 29)/SC

L30 7 S L27 AND (25 OR 27)/SC,SX

L31 1 S L30 NOT L28
SEL RN L29

FILE 'REGISTRY' ENTERED AT 10:42:08 ON 28 FEB 2004

L32 91 S E93-E183

L33 66 S L32 AND NR>=2

FILE 'HCAPLUS' ENTERED AT 10:43:21 ON 28 FEB 2004

L34 1163 S L27 NOT L28-L31

L35 2 S L34 AND LIBRARY

L36 2 S L34 AND COMBINATOR?

L37 3 S L34 AND SOLID PHASE

L38 7 S L35-L37

L39 1 S L34 AND 21/SC,SX

L40 1 S L34 AND HIGH THROUGHPUT

L41 0 S L34 AND HIGH THROUGH PUT

L42 0 S L34 AND HTS

L43 13 S L34 AND SCREEN?

L44 1 S L40 AND L43

L45 0 S L34 AND SCAFFOLD?

L46 12 S L34 AND ?ARRAY?

FILE 'REGISTRY' ENTERED AT 10:47:54 ON 28 FEB 2004

FILE 'HCAPLUS' ENTERED AT 10:48:06 ON 28 FEB 2004

FILE 'USPATFULL, USPAT2' ENTERED AT 10:48:36 ON 28 FEB 2004

FILE 'HCAPLUS' ENTERED AT 10:48:56 ON 28 FEB 2004

SET COST ON

SET COST OFF

FILE 'REGISTRY' ENTERED AT 10:49:40 ON 28 FEB 2004

E C12H11N/MF

L47 113 S E3 AND 46.150.18/RID AND 2/NR

L48 16 S L47 AND BENZENAMINE

L49 1 S 122-39-4

L50 E C13H10O2/MF
L51 149 S E3 AND 46.150.18/RID AND 2/NR
L52 4 S L50 AND BENZOIC ACID AND ESTER
 1 S 93-99-2
 E C13H12O/MF
L53 298 S E3 AND 46.150.18/RID
L54 182 S L53 AND 2/NR
L55 136 S L54 NOT (C5 OR OC4)/ES
L56 115 S L55 NOT ONE
L57 99 S L56 NOT HYDROXY
L58 46 S L57 NOT OL
L59 5 S L58 AND PHENOXYMETHYL
L60 1 S 946-80-5
L61 3 S L49,L52,L60

FILE 'REGISTRY' ENTERED AT 10:54:01 ON 28 FEB 2004

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